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Effect of Electronic Correlation on Atomic Excitation Probability Accompanying β Decay

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The probability of atomic excitation for K-shell electron during nuclear β decay has been calculated on the basis of the sudden approximation. Calculations were made with the variational wave functions for the ground states of helium isoelectronic sequence. The effect of electronic correlation on atomic excitation probability is discussed.

KEY WORDS: β decay / Atomic excitation / Electronic correlation effect /

I. INTRODUCTION

During the β decay of the radioactive nuclides, the atomic electrons have a small probability to be excited to an unoccupied bound state or ionized to the continuum. Since the pioneering work of Feinberg[1] and Migdal,[2] this phenomenon has been extensively studied both theoretically and experimentally.[3] Within the framework of the sudden approximation, this process can be understood as the imperfect overlap of the electronic wave functions due to sudden change in the nuclear change.

In earlier calculations of the atomic excitation probability, the hydrogenic wave functions were used. Later Carlson *et al.*[4] made extensive calculations for various atomic shells of the elements from $Z=2$ to 92 with the use of self-consistent-field (SCF) wave functions. However, all these calculations are based on the single-electron approximation and neglect the electronic correlation effect in the atoms.

The first theoretical investigation with wave functions including electronic correlation was made by Winther.[5] He calculated the atomic excitation probability in the β decay of ^{6}He by the use of the Hylleraas-type wave functions. Similar calculations have also been made for ^{6}He by Kołos[6] and for H^+ and He by Skorobogatov.[7] Their calculations, however, are limited to the small atomic numbers less than 3. Since the existence of another K-shell electron plays an important role to determine the behavior of a K-shell electron in a complex atom, two-electron wave function corresponding to the ground states of helium-like atom can be considered to be a good approximation to the K-shell wave function in many-electron atom. It is interesting to evaluate the atomic excitation probability accompanying β decay of higher-Z nuclides by using the two-electron wave functions including correlation effect.

It is the purpose of the present work to calculate the atomic excitation probability in nuclear β decay of helium-like atoms and estimate the electronic correlation effect

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on the atomic excitation probability.

II. EXCITATION PROBABILITY

We shall consider the atomic excitation probability accompanying β^- decay of helium-like atoms. In the sudden approximation, the probability of the atomic electron initially in its ground state of the atomic number Z to be found in a final state n (discrete or continuum) is given by

$$P_{0n}=|<\psi_n(Z+1)|\psi_K(Z)>|^2, \tag{1}$$

where $\psi_K(Z)$ and $\psi_n(Z+1)$ are the two-electron wave functions of the initial and final states, respectively.

When the final state is also the ground state of the daughter atom with the atomic number $Z+1$, Eq. (1) corresponds to the probability of finding the two electrons in the K shell of the daughter atom:

$$P_{00}=|<\psi_K(Z+1)|\psi_K(Z)>|^2. \tag{2}$$

Since the probability defined in Eq. (1) fulfills the condition

$$\sum_n P_{0n}=1, \tag{3}$$

the atomic excitation probability for removing a K-shell electron to higher states (discrete or continuum) is expressed as

$$P=1-P_{00}. \tag{4}$$

If we neglect the effect of electronic correlation, the wave function $\psi_K(Z)$ is given as the product of two single-electron wave functions:

$$\psi_K(Z)=\phi_K^{(1)}(Z)\phi_K^{(2)}(Z), \tag{5}$$

where $\phi_K^{(i)}(Z)$ is a single-electron wave function for the K-shell electron in the atom with the atomic number Z. The excitation probability is given by

$$P'=1-P_0, \tag{6}$$

where P_0 is defined as

$$P_0=|<\phi_K(Z+1)|\phi_K(Z)>|^4. \tag{7}$$

III. OVERLAP INTEGRALS

From Eqs. (4) and (7), the atomic excitation probability accompanying β decay can be calculated by the use of overlap integrals of the wave functions for K-shell electrons in the initial and final states.

For two-electron wave functions with correlation, we used the Hylleraas-type wave function:[8]

$$\psi_K(Z)=N_0\exp(-ks/2)(1+c_1ku+c_2k^2t^2), \tag{8}$$

where $s=r_1+r_2$, $t=r_1-r_2$, $u=r_{12}$, r_1 and r_2 are the coordinates of two electrons with

respect to the nucleus, and r_{12} is the interelectronic separation distance. All the parameters in Eq. (8) are given in Ref. 8 as a simple function of atomic number Z.

On the other hand, the single K-shell electron wave function is given by

$$\phi_K(Z)=\frac{\zeta^{3/2}}{\pi^{1/2}}\exp(-\zeta r), \tag{9}$$

where ζ is the effective nuclear charge. In the case of hydrogenic wave function, ζ is taken to be Z. When we neglect the electronic correlation effect in the two-electron wave function, ζ can be determined by the variational method as

$$\zeta=Z-\frac{5}{16}, \tag{10}$$

and this corresponds to the screened hydrogenic model.

The overlap integral for the correlated wave function [Eq. (8)] is expressed as

$$M=<\psi_K(Z+1)|\psi_K(Z)>. \tag{11}$$

The integrations with respect to three variables (s, t, and u) can be performed straightforward and the result is given by

$$\begin{aligned}M=2\pi^2N_0N_0'\{&32+140(c_1k+c_1'k')/a+192(c_2k^2+c_2'k'^2)/a^2\\&+1232(c_1c_2'kk'^2+c_2c_1'k^2k')/a^3+768c_1c_1'kk'/a^2\\&+4608c_2c_2'k^2k'^2/a^4\}/a^6,\end{aligned} \tag{12}$$

where $a=(k+k')/2$ and the primed quantities refer to the parameters for $Z+1$.

For the hydrogenic and screened hydrogenic wave functions [Eq. (9)], the overlap integral is easily given by

$$\begin{aligned}M'&=<\phi_K(Z+1)|\phi_K(Z)>\\&=8(\zeta\zeta')^{3/2}/(\zeta+\zeta')^3.\end{aligned} \tag{13}$$

IV. RESULTS AND DISCUSSION

The calculations of the atomic excitation probability accompanying β decay, P, have been made by the use of Eqs. (2), (4), and (12), while the excitation probability in the single-electron approximation, P', was evaluated from Eqs. (6), (7), and (13). The two P' values were calculated. In the first case, called the screened hydrogenic model, ζ is chosen to be $Z-5/16$. This corresponds to neglection of the electronic correlation effect. In the second case, called the hydrogenic model, ζ is equal to Z. This is the case where both electronic correlation and mutual screening between two K-shell electrons are neglected. All the calculations have been performed with the FACOM M-200 computer in the Data Processing Center of Kyoto University.

In Table I we compare the calculated values of the atomic excitation probability in β decay of He. The upper part of the table represents the results obtained by taking into account the electronic correlation. The values without correlation effect, P', are listed in the lower part. Comparing the values with and without correlation effect, it is clear that all the single-electron wave functions give a smaller probability. This fact has been already pointed out by Kołos.[6] The hydrogenic model gives the

Table I. Comparison of the Atomic Excitation Probability in the β Decay of He

	P
Winther[5]	0.3302
Kołos[6]	0.3141
Skorobogatov[7]	0.28991
Present work	0.2932
Hydrogenic ($\zeta=Z$)	0.2172
Screened hydrogenic ($\zeta=Z-5/16$)	0.2753
Weiss[9]	0.2686
Carlson *et al.*[4]	0.269

smallest value and this is the least accurate one. Even the value of Carlson *et al.*[4] calculated by the more accurate SCF wave functions is about 8% smaller than the present result. Weiss[9] calculated the SCF wave functions in the form of expansions in terms of the Laguerre polynomials. His wave functions yield the result in good agreement with the value of Carlson *et al.* The value obtained from the screened hydrogenic model is also close to the SCF values. These facts indicate that for the He atom the electronic correlation effect is essential and increases the atomic excitation probability by about 10%.

On the other hand, there is slight difference between the values with correlation effect. Winther[5] used the 6-parameter function for the ground state of He and the 9-parameter Hylleraas wave function for the Li^+ ion. His result is about 10% larger than other values. However, Skorobogatov[7] claimed that the Hylleraas wave function used by Winther contains very rough approximation and cannot be used in the small-Z region. The largeness of his value is ascribed to this approximation. Kołos[6] tested several simple wave functions with the electronic correlation. His value listed in Table I was obtained by the use of the 3-parameter function for He, but for Li^+ he used less accurate 2-parameter wave function.

The systematic study for the effect of the employed wave functions on the atomic excitation probability has been made by Skorobogatov.[7] For the wave function of the ground state of the He atom, he used the 3-, 5-, 6-, and 10-parameter variational wave functions, while the 3-, 4-, 5-, 9-, and 10-parameter wave functions were used for the Li^+ ion. For various combinations of the wave functions of the He and Li^+ atoms, the atomic excitation probabilities were calculated and the most reliable value was estimated to be $P=0.28991$ calculated by the 10-parameter wave functions for He and Li^+. It can be seen from Table I that the present value is in good agreement with the value of Skorobogatov. We can say, therefore, that the present wave function [Eq. (8)] is sufficiently accurate even though it contains only three parameters.

In order to estimate the electronic correlation effect on the atomic excitation probability in β decay of other helium-like atoms, the similar calculations have been performed for the atomic numbers from $Z=2$ to 82. In Table II the values calculated

Table II. Comparison of the Atomic Excitation Probabilities in β Decay Calculated in Hydrogenic Model, Screened Hydrogenic Model, the Present Model, and the SCF Model (Probability given in %)

Z	Atom	Hydrogenic ($\zeta=Z$)	Screened hydrogenic ($\zeta=Z-5/16$)	Present model	SCF[4]
2	He	21.72	27.53	29.32	26.9
3	Li	11.64	13.88	14.45	
6	C	3.498	3.885	3.925	2.74
10	Ne	1.353	1.437	1.452	1.03
16	S	0.5497	0.5711	0.5747	0.337
28	Ni	0.1845	0.1886	0.1892	0.115
38	Sr	0.1012	0.1028	0.1030	0.0654
46	Pd	0.06935	0.07029	0.07032	0.0459
62	Sm	0.03839	0.03878	0.03873	0.0282
74	W	0.02702	0.02725	0.02718	0.0225
80	Hg	0.02315	0.02333	0.02325	0.0210
82	Pb	0.02204	0.02220	0.02213	0.0206

by the correlated wave functions are compared with the values obtained from the single-electron wave functions; hydrogenic model ($\zeta=Z$) and screened hydrogenic model ($\zeta=Z-5/16$). It is clear that the hydrogenic model considerably underpredicts the atomic excitation probability of low-Z atoms, but the difference becomes smaller for high-Z atoms. For low-Z atoms the screened hydrogenic model also underpredicts the probability, but gives better values than the hydrogenic model. In the case of $Z>10$ the values obtained from the screened hydrogenic model are in agreement with those calculated by the present correlated wave functions. This fact leads to an interesting conclusion that the correlation effect is important in the region of small Z, but influence of the mutual screening is more dominant.

In order to demonstrate this situation more clearly, the relative deviation of P' from P, $(P-P')/P$, is plotted in Fig. 1 as a function of Z. The solid curve denotes the effect of neglection of electronic correlation, *i.e.*, the screened hydrogenic model ($\zeta=Z-5/16$), and the dashed curve represents the effect of neglection of both electronic correlation and mutual screening, *i.e.* the hydrogenic model ($\zeta=Z$). It can be seen from the figure that the electronic correlation is important only for the small Z values and becomes negligible for $Z>10$. The screening effect reduces the atomic excitation probability of small-Z atoms to a larger extent. This effect also decreases with increasing Z and becomes less than 1% for $Z>40$.

In Table II the atomic excitation probabilities calculated with the SCF wave functions by Carlson *et al.*[4] are listed for comparison. Their values are based on the formula

$$P'=1-P_0-P_F, \tag{14}$$

where P_F is the probability of electron excitation to occupied states, which is forbidden by the Pauli principle. They used nonrelativistic Hartree-Fock wave functions for

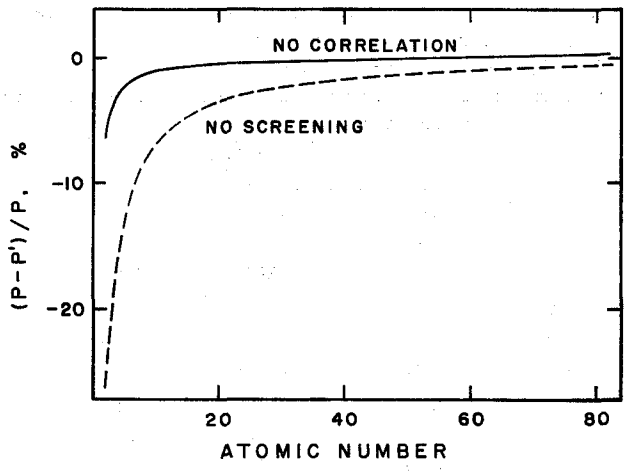

Fig. 1. The effect of electronic correlation on the atomic excitation probability in β decay. Relative difference between the probabilities with and without correlation effect is shown in % and plotted against atomic number. The solid curve represents the difference for the case of no correlation effect ($\zeta=Z-5/16$) and the dahsed curve is that for the case of no correlation effect and no screening effect ($\zeta=Z$).

$Z<30$ and relativistic Hartree-Fock-Slater wave functions for $Z\geq 30$.

It is clear from the table that the SCF values are systematically smaller than the values obtained from the present model. However, except for the case of He ($Z=2$), comparison between two models is not so simple. We must take into consideration two effects in addition to the electronic correlation. First, in the present model we are concerned with only two K-shell electrons in the atoms, while the SCF wave functions are calculated by taking into account existence of the outer-shell electrons. Owing to this outer-shell electron effect, the shape of the K-shell electron wave functions in the SCF model is different from that in the two-electron atoms. Second, in the present model there are only two K-shell electrons in the atom and all the other shells are vacant. This corresponds to $P_F=0$ in Eq. (14) [Eq. (6)]. On the other hand, in the ordinary atoms except for He there exist occupied shells in addition to the K shell and $P_F\neq 0$. As can be seen from Eq. (14), this effect reduces the atomic excitation probability.

Considering these facts, direct comparison between the present model and the SCF model is not conclusive, because the former model gives the atomic excitation probability in β decay of the ground state of the helium-like ions and the latter yields that of the ordinary atoms. However, correction for the electronic correlation effect in the case of the ordinary atoms can be made by multiplying the SCF values by a factor P/P' with $\zeta=Z-5/16$.

V. CONCLUSION

The atomic excitation probability in β decay has been calculated by the use of

the variational wave functions for helium-like atoms. The effect of the electronic correlation has been studied by comparing the calculated probabilities with and without correlation effect. It is found that the correlation effect increases the atomic excitation probability for small-Z atoms. The increase in the probability is about 8% for the He atom. The effect decreases with increasing Z and becomes negligible for $Z>10$. The screening effect is also shown to be important in the small-Z region and exhibits the larger Z dependence than the correlation effect. For the atomic numbers less than 10, both effects should be taken into account to estimate the atomic excitation probability in β decay.

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